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Breaking the Chirality Lock: Theory-Guided Electric-Field Reversal of a Unidirectional Molecular Motor

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Abstract:

Light-driven rotary motors allow direct transformation of light energy into unidirectional rotary motion at the nanoscale, giving rise to countless emerging applications in molecular engineering. The key feature enabling the unidirectional rotation and controlling its direction is the motor chirality, an inherently chemical factor, hard to modify postsynthetically. [1-3]

Here we propose a new molecular rotary motor architecture, E-motor, in which the motor operation direction can be switched in situ, without the need for chemical modification of the system structure. [4] This effect is achieved by the application of an external electric-field pulse and is intended to provide means for chirality control in motors deposited on a surface (Fig. 1a.). Our study relies on quantum-chemical calculations and nonadiabatic molecular dynamics simulations performed for a specifically tailored system, PFCN (Fig.1b.), designed to provide illustration for the proposed new motor type. We show that the model system's chirality and, hence, its operation direction, depends on orientation of a covalently bound polar switching unit, which can be controlled with an external electric field. At the same time, the proposed system manifests all characteristic photophysical properties of a unidirectional molecular motor, and its set chirality is preserved, i.e., it is thermally and optically stable during the regular motor operation in the absence of the electric field.

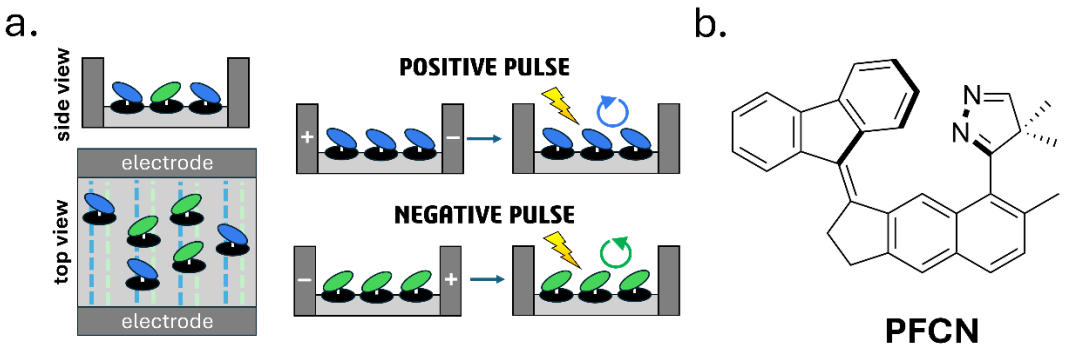

Figure 1. a. Working principle of an array of electric-field controlled molecular rotary motors. b. Electric-field switchable motor structure.

References:

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